

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

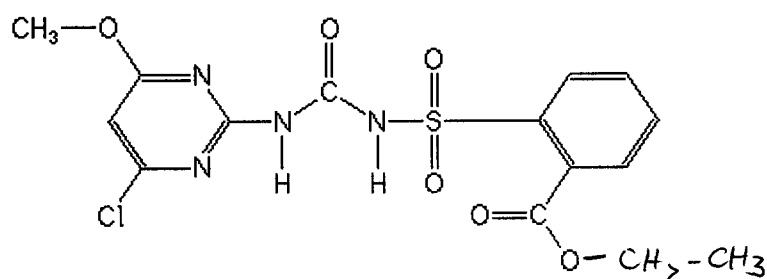
Analyte: Chlorimuron-ethyl

CAS No.: 99283-00-8

Formula: C₁₅H₁₅ClN₄O₆S

Molecular mass (lowest isotopes): 414,04 amu

Structure:



Ionisation: ESI +

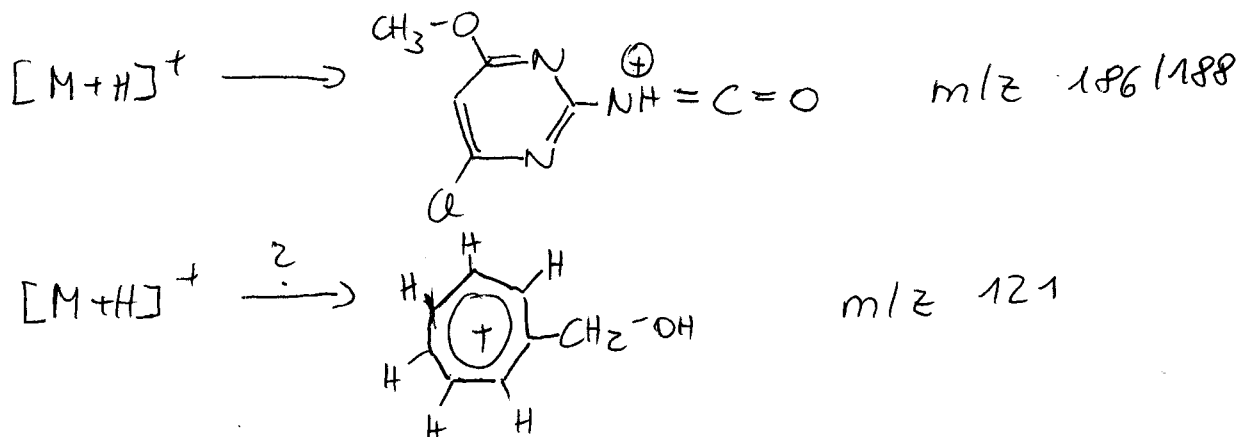
Quasimolecular ion: 415,0 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	415,0 → 121,1	415,0 → 186,1
Declustering potential (DP) ^{*)}	54V	54 V
Focusing potential (FP)	370 V	320 V
Entrance potential (EP)	10 V	10,5 V
Collision cell entrance potential (CEP)	26 V	24 V
Collision energy (CE)	53 V	27 V
Collision cell exit potential (CXP)	6 V	10 V

^{*)} For API 3000 and 4000 enhance DP by 20V

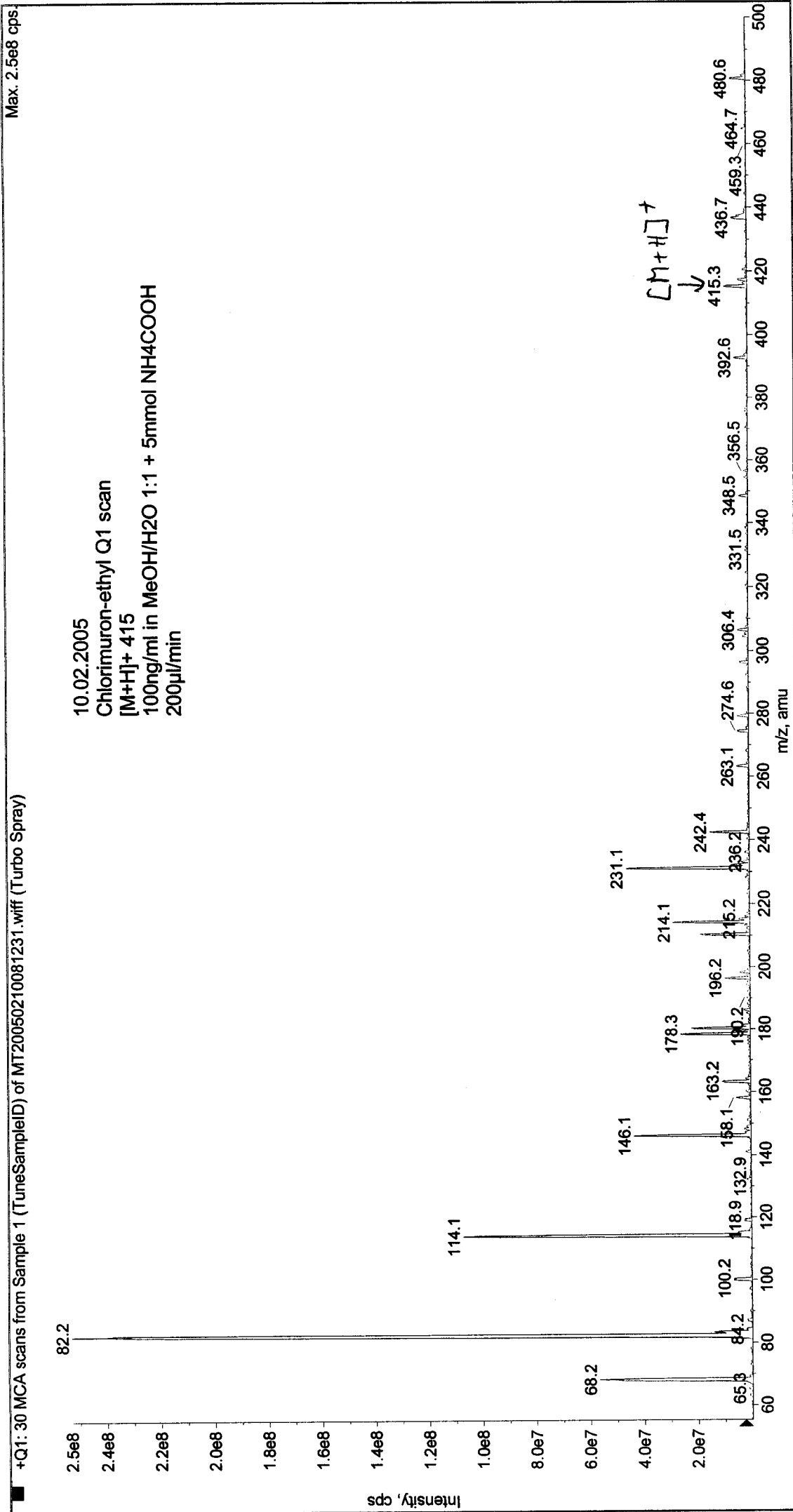
Fragmentation



Printing Time: 8:15:07
Printing Date: Thursday, February 10, 2005

Acq. Time: 08:12
Acq. Date: Thursday, February 10, 2005
Acq. File: MT20050210081231.wiff

Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 8:17:08

Printing Date: Thursday, February 10, 2005

Acq. Time: 08:16

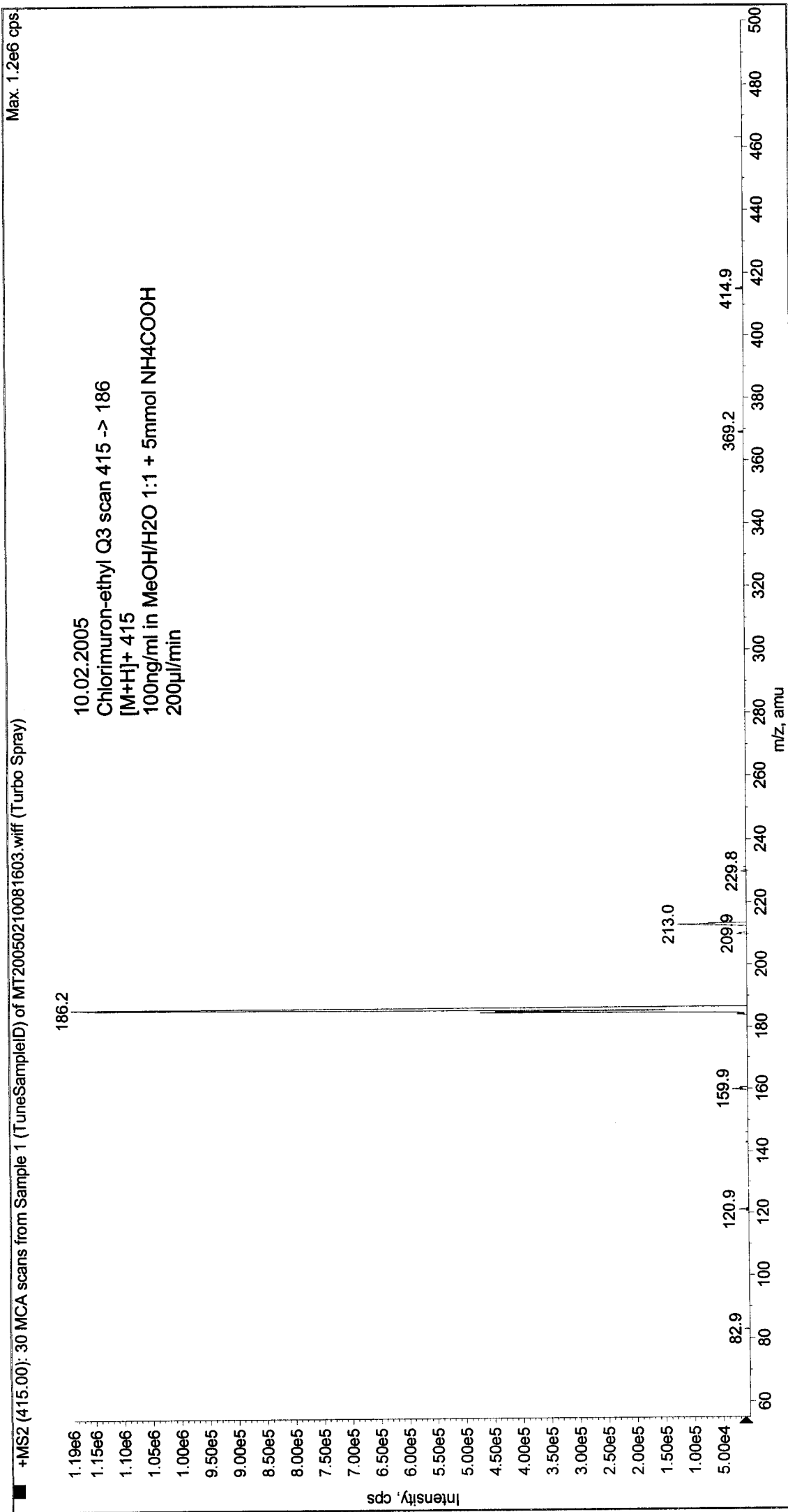
Acq. Date: Thursday, February 10, 2005

Acq. File: MT20050210081603.wiff

Sample Comment:

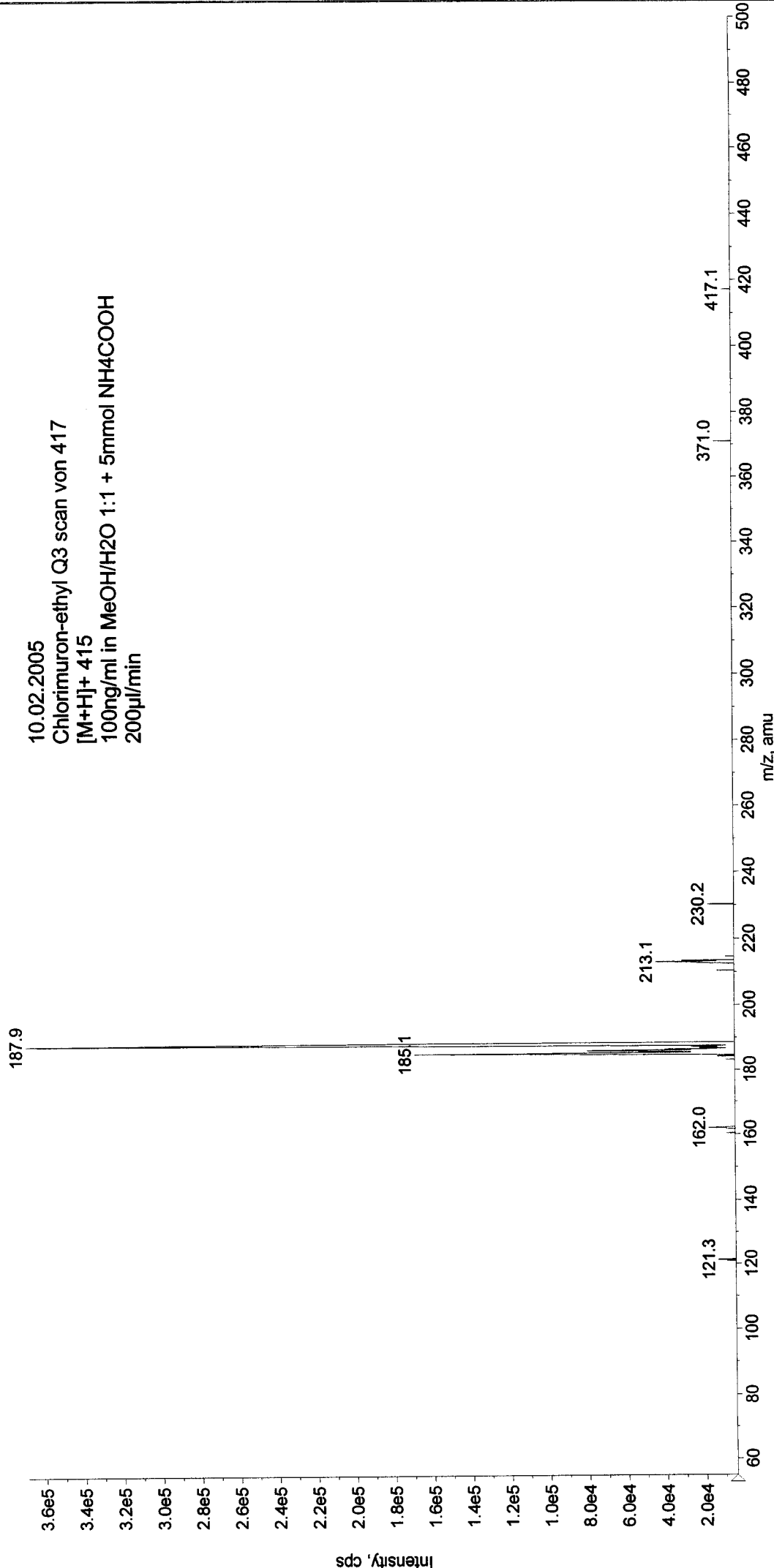
Sample Name: TuneSampleID

Batch Name: ManualTune.bat



+MS2 (417.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050210081727.wiff (Turbo Spray)

10.02.2005
Chlorimuron-ethyl Q3 scan von 417
[M+H]⁺ 415
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



Printing Time: 8:36:20

Printing Date: Thursday, February 10, 2005

Acq. Time: 08:35

Acq. Date: Thursday, February 10, 2005

Acq. File: MT20050210083505.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

Max. 4.3e5 cps

+MS2 (415.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050210083505.wiff (Turbo Spray)

10.02.2005
Chlorimuron-ethyl_121 Q3 scan 415 -> 121
[M+H]⁺ 415
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min

